

Functional renormalization-group approaches, one-particle (ir)reducible with respect to local Green functions, using the dynamical mean-field theory as a starting point

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Abstract

We consider formulations of the functional renormalization-group flow for correlated electronic systems, having the dynamical mean-field theory as a starting point. We classify the corresponding renormalization-group schemes into those neglecting the one-particle irreducible (with respect to the local Green functions) six-point vertices and neglecting one-particle reducible six-point vertices. The former class is represented by the recently introduced DMF²RG approach [Phys. Rev. Lett. **112**, 196402 (2014)], but also by the scale-dependent generalization of the one-particle irreducible (with respect to local Green functions, 1PI-LGF) representation of the generating functional [Phys. Rev. B **88**, 115112 (2013)]. The second class is represented by the fRG flow within the dual fermion (DF) approach [Phys. Rev. B **77**, 033101 (2008); ArXiv 1411.1342]. We compare formulations of fRG approach in each of these cases and suggest their further application to study 2D systems within the Hubbard model.

I. INTRODUCTION

Strongly correlated electron systems demonstrate a variety of interesting phenomena, such as magnetism, (unconventional) superconductivity, “colossal” magnetoresistance, and quantum critical behavior. The dynamical mean-field theory (DMFT)[1, 2], which becomes exact in the limit of high spatial dimensions ($d \rightarrow \infty$), allowed to achieve a substantial progress in describing strong electronic correlations. In particular it allowed to describe accurately the Mott-Hubbard metal-insulator transition[3] due to account of an important local part of electronic correlations.

In real physical systems, which are one-, two-, or three-dimensional, the nonlocal correlations, which are neglected in DMFT, are, however, important. Cluster extensions of DMFT [4–8] can treat only short-range correlations due to numerical limitations of the cluster size[9]. In spite of this, the diagrammatic extensions of the dynamical mean-field theory were developed. These are the dynamical vertex approximation (DFA) [10–15], the dual fermion (DF) approach [16–19], and the one-particle irreducible with respect to the local Green functions (1PI-LGF) approach [20]. The former approximation starts from the local two-particle irreducible vertices and sums ladder or parquet diagrams for the vertex, considering the effect of the non-locality of the Green functions. The DF approach on the other hand splits the degrees of freedom into the local ones, treated within DMFT, and the non-local (dual) degrees, considered perturbatively, with a possibility of summation of infinite series of diagrams for dual fermions [19, 21]. The 1PI version of the dual fermion approach (the 1PI-LGF approach) performs the same splitting of the local and non-local degrees of freedom for 1PI (Legendre-transformed) generating functionals. This approach accounts therefore for the effect of one-particle reducible six-point and higher-order reducible vertices, which was argued to be of possible importance in Ref. [33].

The abovediscussed approaches typically treat non-local fluctuations within the ladder approximation. More powerful method - parquet approach can bring substantial improvement over the ladder approximation[21, 22], but often not accessible numerically for correlated electronic systems. At the same time, recently developed functional renormalization group (fRG) approaches [23–28] allow for lower computational cost perform approximate summation of the parquet set of the diagrams, provided that the six-point (i.e. three-particle) interaction vertices remain sufficiently small during the flow. In particular, for the standard

fRG, applied to the Hubbard model, the initial particle irreducible six-point vertices are zero, which advances using the one-particle irreducible approach, in which one can expect that the corresponding six-point vertex remain small during the flow. Using the dynamical mean-field theory as an initial theory for the flow account exactly for the local subset of diagrams, but yields (in principle) non-zero vertices up to infinite order, so that the formulation and justification of the fRG approach requires more effort. In general, in this case, one has a choice between neglecting the six-point one-particle *irreducible* or *reducible* vertices, which depends on considering model. In particular, in the half-filled spinless Falikov-Kimball model the one-particle reducible six-point local vertex vanishes in the infinite-dimensional limit [29], while for the Hubbard model, at least in the weak-to-intermediate coupling limit, neglecting six-point one-particle irreducible local vertices seems more preferable.

In the present paper we concentrate on the renormalization-group approaches, which use dynamical mean-field theory as a starting point, and neglect either one-particle irreducible or one-particle reducible (with respect to the local Green function) three-particle vertices (see also Ref. [30]). Recently, an approach of the former type, considering the functional renormalization-group flow from infinite to finite dimensions (the DMF²RG approach) was introduced[31]. This flow starts from infinite-dimensional model, which is solved by DMFT, and considers the flow to finite number of dimensions, e.g. in the approximation of neglecting the local six-point vertices. Because of the using 1PI approach, the latter approximation implies neglect of the six-point vertices, which are one-particle *irreducible* with respect to the local Green functions. To have more general view on the possible variety of different renormalization-group approaches, starting from the dynamical mean-field theory, it is informative to formulate the fRG approach for the other two mentioned schemes, i.e. 1PI-LGF and DF theories, and compare them to the DMF²RG approach. This study is performed in the present paper.

II. THE MODEL AND DYNAMICAL MEAN-FIELD THEORY

We consider general one-band model of fermions, interacting via local interaction $H_{\text{int}}[\hat{c}_{i\sigma}, \hat{c}_{i\sigma}^+]$

$$H = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma}^+ \hat{c}_{\mathbf{k}, \sigma} + \sum_{i, \sigma} H_{\text{int}}[\hat{c}_{i\sigma}, \hat{c}_{i\sigma}^+], \quad (1)$$

where $\widehat{c}_{i\sigma}, \widehat{c}_{i\sigma}^+$ are the fermionic operators, and $\widehat{c}_{\mathbf{k},\sigma}, \widehat{c}_{\mathbf{k},\sigma}^+$ are the corresponding Fourier transformed objects, $\sigma = \uparrow, \downarrow$ corresponds to a spin index. The model is characterized by the generating functional

$$Z[\eta, \eta^+] = \int d[c, c^+] \exp \{ -\mathcal{S}[c, c^+] + \eta^+ c + c^+ \eta \} \quad (2)$$

$$\mathcal{S}[c, c^+] = \int d\tau \left\{ \sum_{i,\sigma} c_{i\sigma}^\dagger(\tau) \frac{\partial}{\partial \tau} c_{i\sigma}(\tau) + H[c, c^+] \right\} \quad (3)$$

where $c_{i\sigma}, c_{i\sigma}^+, \eta_{i\sigma}, \eta_{i\sigma}^+$ are the Grassman fields, the fields $\eta_{i\sigma}, \eta_{i\sigma}^+$ correspond to source terms, $\tau \in [0, \beta = 1/T]$ is the imaginary time. The dynamical mean-field theory [1, 2] for the model (1) can be introduced via effective interaction

$$\begin{aligned} \mathcal{V}_{\text{DMFT}}[\eta, \eta^+] = & -\ln \int d[c, c^+] \exp \left\{ -\sum_{i,\sigma} \int d\tau H_{\text{int}}[c_{i\sigma}, c_{i\sigma}^+] \right. \\ & \left. + \sum_{k,\sigma} \zeta^{-1}(i\nu_n) (c_{k,\sigma}^+ + \eta_{k,\sigma}^+)(c_{k,\sigma} + \eta_{k,\sigma}) \right\} \end{aligned} \quad (4)$$

where the "Weiss field" function $\zeta(\tau)$ and its Fourier transform $\zeta(i\nu_n)$ has to be determined self-consistently from the condition

$$G_{\text{loc}}(i\nu_n) \equiv \frac{1}{\zeta^{-1}(i\nu_n) - \Sigma_{\text{loc}}(i\nu_n)} = \sum_{\mathbf{k}} \mathcal{G}(\mathbf{k}, i\nu_n), \quad (5)$$

where

$$\mathcal{G}(\mathbf{k}, i\nu_n) \equiv \mathcal{G}_k = [G_{0k}^{-1} - \Sigma_{\text{loc}}(i\nu_n)]^{-1}, \quad (6)$$

$G_{0k}^{-1} = i\nu_n - \varepsilon_{\mathbf{k}}$ is the lattice noninteracting Green function (we use the 4-vector notation $k = (\mathbf{k}, i\nu_n)$) and $\Sigma_{\text{loc}}(i\nu_n)$ is the self-energy of the impurity problem (4), which is in practice obtained within one of the impurity solvers: exact diagonalization, quantum Monte-Carlo, etc. These solvers provide information not only on the electronic self-energy, but also the corresponding vertex functions[10, 32]. This is reflected in the following expansion of the effective interaction:

$$\mathcal{V}_{\text{DMFT}}[\eta, \eta^+] = \widehat{\mathcal{V}}_{\text{DMFT}}[\widehat{\eta}_{k\sigma}, \widehat{\eta}_{k\sigma}^+] + \sum_{k,\sigma} \eta_{k,\sigma}^+ \frac{\Sigma_{\text{loc}}(i\nu_n)}{1 - \zeta(i\nu_n)\Sigma_{\text{loc}}(i\nu_n)} \eta_{k,\sigma}, \quad (7)$$

where $\widehat{\eta}_{k,\sigma} = \eta_{k\sigma}/(1 - \Sigma_{\text{loc}}(i\nu_n)G_{0k})$. The functional $\widehat{\mathcal{V}}_{\text{DMFT}}[\eta, \eta^+]$ generates connected vertices (which are in general one-particle reducible), amputated by the local Green function

$G_{\text{loc}}(i\nu_n)$, such that its expansion in fields reads

$$\begin{aligned}\widehat{\mathcal{V}}_{\text{DMFT}}[\eta^+, \eta] &= \frac{1}{2}\Gamma_{\text{loc}} \circ (\eta_{k_1, \sigma}^+ \eta_{k_3, \sigma})(\eta_{k_2, \sigma'}^+ \eta_{k_4, \sigma'}) \\ &\quad + \frac{1}{6}\Gamma_{\text{loc}}^{(6)} \circ (\eta_{k_1, \sigma}^+ \eta_{k_2, \sigma})(\eta_{k_3, \sigma'}^+ \eta_{k_4, \sigma'})(\eta_{k_5, \sigma''}^+ \eta_{k_6, \sigma''}) + \dots\end{aligned}\quad (8)$$

where Γ_{loc} and $\Gamma_{\text{loc}}^{(6)}$ are the connected 4- and 6-point vertices, amputated with the local Green functions G_{loc} , e.g.

$$\begin{aligned}\widetilde{\Gamma}_{\text{loc}}^{\sigma\sigma'}(i\nu_1..i\nu_3) &= (1 + \delta_{\sigma\sigma'})^{-1} \prod_{i=1}^4 G_{\text{loc}}^{-1}(i\nu_i) \\ &\quad \times \left[G_{\text{loc}, \sigma\sigma'}^{(4)}(i\nu_1..i\nu_3) - G_{\text{loc}}(i\nu_1)G_{\text{loc}}(i\nu_2)(\delta_{\nu_1\nu_3} - \delta_{\sigma\sigma'}\delta_{\nu_2\nu_3}) \right],\end{aligned}\quad (9)$$

and \circ stands for summation over momenta- frequency- and spin indices fulfilling the conservation laws, $G_{\text{loc}}^{(4)}$ is the two-particle local Green function, which can be obtained via the solution of the impurity problem. For the four-point vertex Γ_{loc} the requirement of connectivity and amputation with the full local Green functions implies one-particle irreducibility. However, the higher-order vertices, e.g. $\Gamma_{\text{loc}}^{(6)}$ remain one-particle reducible with respect to the local Green functions. To obtain the one-particle irreducible vertices, Legendre transformation of Eq. (4) has to be performed.

III. THE ONE-PARTICLE IRREDUCIBLE APPROACHES WITH RESPECT TO LOCAL GREEN FUNCTIONS

A. The flow from infinite to finite dimension within the DMF²RG approach

Recently, in Ref. [31] the flow from infinite to finite number of dimensions was introduced. This flow considers evolution of generating functional with the action

$$\mathcal{S}_\Lambda = \sum_{k\sigma} c_{k\sigma}^+ G_{0k, \Lambda}^{-1} c_{k\sigma} + \sum_{i, \sigma} \int d\tau H_{\text{int}}[c_{i\sigma}, c_{i\sigma}^+] \quad (10)$$

with the cutoff dependence of the bare Green function

$$G_{0k, \Lambda} = 1/[f(k, \Lambda)G_{0, k}^{-1} + (1 - f(k, \Lambda))\zeta^{-1}(i\nu_n)] \quad (11)$$

with some function $f(k, \Lambda)$, such that $f(k, 1) = 0$ and $f(k, 0) = 1$; specific choices of this function are discussed in Sect. IV ($f(k, \Lambda) = 1 - \Lambda$ was used in Ref. [31]). The 1PI approach,

applied to the model (10) yields equations

$$\frac{d\Sigma_\Lambda}{d\Lambda} = V_\Lambda \circ S_\Lambda, \quad (12)$$

$$\frac{dV_\Lambda}{d\Lambda} = V_\Lambda \circ (G_\Lambda \circ S_\Lambda + S_\Lambda \circ G_\Lambda) \circ V_\Lambda, \quad (13)$$

where

$$G_{k,\Lambda} = G_{0k,\Lambda} / [1 - \Sigma(k, \Lambda) G_{0k,\Lambda}], \quad (14)$$

$$S_{k,\Lambda} = \left. \frac{dG_{k,\Lambda}}{d\Lambda} \right|_{\Sigma=\text{const}} = -(\mathcal{G}_k^{-1} - G_{\text{loc}}^{-1}) \frac{\partial f}{\partial \Lambda} G_{k,\Lambda}^2. \quad (15)$$

This approach uses initial one-particle irreducible vertices and self-energy as an initial condition for the flow: $V_{\Lambda=1} = \Gamma_{\text{loc}}^{\uparrow\downarrow}$, $\Sigma_{\Lambda=1} = \Sigma_{\text{loc}}$, which are in practice obtained from the solution of the AIM. At the same time, equations (12) and (13) neglect local 1PI six-point vertex at the initial stage of the flow.

B. General formulation of the 1PI-LGF approach

Another way of the treatment of non-local correlations, based on the dynamical mean-field theory as a starting point, is splitting of the local and non-local correlations in the generating functional for lattice theory. For one-particle irreducible version, this was done within the 1PI-LGF approach, considered in Ref. [20]. This approach represents the partition function as a functional of the local Green function G_{loc} and the corresponding non-local part $\tilde{\mathcal{G}}_k = \mathcal{G}_k - G_{\text{loc}}$. Contrary to the dual fermion approach, considered in the next Section, this representation contains two fermionic fields, one of which describes propagation of non-local degrees of freedom (similarly to the DF approach), while the other one provides one-particle irreducibility of the resulting functional.

To formulate the renormalization-group treatment within this approach, we generalize trivially the representation for the partition function, obtained in Ref. [20], to introduce Λ -dependence of the lattice Green function \mathcal{G}_k by the replacement $\mathcal{G}_k \rightarrow \mathcal{G}_{k,\Lambda}$ where $\mathcal{G}_{k,\Lambda}$ is defined by

$$\mathcal{G}_{k,\Lambda} = 1/[f(k, \Lambda)\mathcal{G}_k^{-1} + (1 - f(k, \Lambda))G_{\text{loc}}^{-1}(i\nu_n)], \quad (16)$$

which is similar to the Eq. (11). The other choice, which we consider below is combining the two Green functions (and not their inverse) in a sum,

$$\mathcal{G}_{k,\Lambda} = f(k, \Lambda)\mathcal{G}_k + [1 - f(k, \Lambda)]G_{\text{loc}}(i\nu_n) \quad (17)$$

such that

$$\tilde{\mathcal{G}}_k \rightarrow \tilde{\mathcal{G}}_{k,\Lambda} := \mathcal{G}_{k,\Lambda} - G_{\text{loc}}(i\nu_n) = f(k, \Lambda)[\mathcal{G}_k - G_{\text{loc}}(i\nu_n)]. \quad (18)$$

The resulting Λ -dependent partition function in both cases reads[20]:

$$\begin{aligned} Z_\Lambda[\eta^+, \eta] = & \int D[\phi^+, \phi] D[\psi^+, \psi] \exp \left\{ \sum_{k,\sigma} \eta_{k\sigma}^+ (\psi_{k\sigma} + \phi_{k\sigma}) + (\psi_{k\sigma}^+ + \phi_{k\sigma}^+) \eta_{k\sigma} \right. \\ & + \frac{1}{\beta} \sum_{k,\sigma} \mathcal{G}_{k,\Lambda}^{-1} (\phi_{k\sigma}^+ \phi_{k\sigma} + \psi_{k\sigma}^+ \phi_{k\sigma} + \phi_{k\sigma}^+ \psi_{k\sigma}) + (\mathcal{G}_{k,\Lambda}^{-1} - G_{\text{loc},\nu}^{-1}) \psi_{k\sigma}^+ \psi_{k\sigma} \\ & - \frac{1}{\beta^3} \sum_{kk'q} \sum_{\sigma\sigma'} \tilde{\Gamma}_{\text{loc},\sigma\sigma'}^{\nu\nu'\omega} [(\psi_{k\sigma}^+ \phi_{k+q,\sigma}) (\phi_{k'+q,\sigma'}^+ \phi_{k'\sigma'}) \\ & \left. + (\phi_{k\sigma}^+ \phi_{k+q,\sigma}) (\phi_{k'+q,\sigma'}^+ \psi_{k'\sigma'}) + \frac{1}{2} (\phi_{k\sigma}^+ \phi_{k+q,\sigma}) (\phi_{k'+q,\sigma'}^+ \phi_{k'\sigma'}) \right] \Big\} J[\phi^+, \phi], \quad (19) \end{aligned}$$

where $J[\phi^+, \phi]$ is the Jacobian, defined in terms of local degrees of freedom in Ref. [20]; $\tilde{\Gamma}_{\text{loc},\sigma\sigma'}^{\nu\nu'\omega} = (1 - \delta_{\sigma\sigma'}/2) \Gamma_{\text{loc},\sigma\sigma'}^{\nu\nu'\omega}$. Eq. (19) contains integration over two fermionic fields ϕ and ψ , the latter appears after fermionic Hubbard-Stratanovich transformation of the Legendre transformation of the action and provides one-particle irreducibility of the resulting approach with respect to the local Green functions. The diagrammatic meaning of Eq. (19), as well as the summation of the ladder diagrams for the vertex and their effect on the self-energy was discussed in details in Ref. [20]; here we consider renormalization-group approach to this representation.

The bare propagator of the representation (19), which includes fully the effect of the local self-energy, can be conveniently written in the spinor representation[20],

$$\Phi_{k\sigma} = \begin{pmatrix} \phi_{k\sigma} \\ \psi_{k\sigma} \end{pmatrix}, \quad (20)$$

and it reads

$$\mathbf{G}_{k,\Lambda} = -\frac{1}{\beta} \langle \langle \Phi_k | \Phi_k^+ \rangle \rangle_0 = \begin{pmatrix} \mathcal{G}_{k,\Lambda}^{-1} & \mathcal{G}_{k,\Lambda}^{-1} \\ \mathcal{G}_{k,\Lambda}^{-1} & \mathcal{G}_{k,\Lambda}^{-1} - G_{\text{loc},\nu}^{-1} \end{pmatrix}^{-1} = \begin{pmatrix} \tilde{\mathcal{G}}_{k,\Lambda} & G_{\text{loc},\nu} \\ G_{\text{loc},\nu} & -G_{\text{loc},\nu} \end{pmatrix}. \quad (21)$$

The corresponding equations for the vertex $\mathbb{V}_\Lambda^{\alpha\beta\gamma\delta}(k_1, k_2; k_3, k_4)$ (k_1, k_2 and k_3, k_4 are the momenta- and frequencies of the incoming and outgoing electrons, $k_i = (\mathbf{k}_i, i\nu_n^{(i)})$, $\alpha, \beta, \gamma, \delta = 1, 2$ correspond to ϕ and ψ fields, respectively) and the non-local part of the self-energy

$\tilde{\Sigma}_\Lambda^{\alpha\beta}(\mathbf{k}, i\nu_n)$ read

$$\frac{d\tilde{\Sigma}_\Lambda}{d\Lambda} = \mathbb{V}_\Lambda \circ \mathbb{S}_\Lambda; \quad (22)$$

$$\frac{d\mathbb{V}_\Lambda}{d\Lambda} = \mathbb{V}_\Lambda \circ (\mathbb{G}_\Lambda \circ \mathbb{S}_\Lambda + \mathbb{S}_\Lambda \circ \mathbb{G}_\Lambda) \circ \mathbb{V}_\Lambda, \quad (23)$$

where

$$\mathbb{G}_{k,\Lambda} = [\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda}]^{-1}. \quad (24)$$

For the choice of the propagators (16) we obtain

$$\mathbb{S}_{k,\Lambda} = -(\mathcal{G}_k^{-1} - G_{\text{loc}}^{-1}) \frac{\partial f(k, \Lambda)}{\partial \Lambda} [\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda}]^{-1} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} [\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda}]^{-1}, \quad (25)$$

while for the propagator (17) we find

$$\mathbb{S}_{k,\Lambda} = -(\mathcal{G}_k - G_{\text{loc}}) \mathcal{G}_{k,\Lambda}^{-2} \frac{\partial f(k, \Lambda)}{\partial \Lambda} [\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda}]^{-1} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} [\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda}]^{-1}. \quad (26)$$

Note that the non-local (physical) Green function can be directly obtained from Eqs. (23) by summing all the components of the matrix Green function $(\mathbf{G}_{k,\Lambda}^{-1} - \tilde{\Sigma}_{k,\Lambda})^{-1}$, the corresponding ‘physical’ self-energy is then extracted in the standard way from the physical Green function and the flowing bare Green function $(\mathcal{G}_{k,\Lambda}^{-1} + \Sigma_{\text{loc}})^{-1}$.

For $\Lambda \geq \Lambda_0$ (Λ_0 is the upper scale of the problem) we have $\tilde{G}_\Lambda = 0$, so that only \mathbf{G}^{12} , \mathbf{G}^{21} , and \mathbf{G}^{22} elements of the Green function are nonzero, which corresponds to a purely local theory. It can be shown that the contribution of these Green functions are exactly compensated by the “counterterms” which arise from the Jacobian of the transformation. The initial conditions for the vertex and the self-energy are

$$\begin{aligned} \mathbb{V}_\Lambda^{1111}(k_1, k_2; k_3, k_4) &= \mathbb{V}_\Lambda^{1211}(k_1, k_2; k_3, k_4) = \mathbb{V}_\Lambda^{2111}(k_1, k_2; k_3, k_4) \\ &= \mathbb{V}_\Lambda^{1121}(k_1, k_2; k_3, k_4) = \mathbb{V}_\Lambda^{1112}(k_1, k_2; k_3, k_4) \\ &= \Gamma_{\text{loc}}^{\uparrow\downarrow}, \end{aligned} \quad (27)$$

$$\tilde{\Sigma}^{\alpha\beta}(k) = 0. \quad (28)$$

C. Comparison to the DMF²RG approach

To compare the fRG flow within 1PI-LGF and DMF²RG approaches, we consider the choice of the propagators (16) and (25). In the following consideration we assume the

following structure of the self-energy correction:

$$\Sigma_{k,\Lambda} = \Sigma_{k,\Lambda}^{(1)} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \Sigma_{k,\Lambda}^{(2)} \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad (29)$$

which was obtained in the ladder approximation in Ref. [20] and justified self-consistently below. With this assumption, the Green function $\mathbb{G}_{k,\Lambda}$ can be represented in the form

$$\mathbb{G}_{k,\Lambda} = G_{k,\Lambda} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{G_{\text{loc},\nu}}{1 - G_{\text{loc},\nu} \Sigma_{k,\Lambda}^{(2)}} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \quad (30)$$

where $G_{k,\Lambda}$ is given by the Eq. (14) with $\Sigma_{k,\Lambda} = \Sigma_{k,\Lambda}^{(1)} + \Sigma_{k,\Lambda}^{(2)}$. For the single-scale propagator we obtain

$$\mathbb{S}_{k,\Lambda} = \begin{pmatrix} S_{k,\Lambda} & 0 \\ 0 & 0 \end{pmatrix}, \quad (31)$$

where $S_{k,\Lambda}$ is identical to the single-scale propagator (15), considered in Ref. [31].

Considering the $\Sigma_{k,\Lambda}^{11} = \Sigma_{k,\Lambda} \equiv \Sigma_{k,\Lambda}^{(1)} + \Sigma_{k,\Lambda}^{(2)}$ component of the self-energy and $\mathbb{V}_{\Lambda}^{1111}(k_1, k_2; k_3, k_4)$ component of the vertex, the first term in Eq. (30) yields the equations of the DMF²RG approach, while the second term yields zero in the assumption that the vertex keeps its structure (27). We have to verify however, that the Eqs. (27) and (31) are preserved by the considering approach. Let consider first the self-energy. Assuming fulfillment of the ansatz for the vertices (27) and using the result (31) for the single-scale propagator, we find $\Sigma_{k,\Lambda}^{11} = \Sigma_{k,\Lambda}^{12} = \Sigma_{k,\Lambda}^{21}$. This implies fulfillment of (31). Let now verify fulfillment of the vertex ansatz (27). Starting with this ansatz and (31), we find that the first term in Eq. (30) yields fulfillment of the first two lines of (27). For the vertices $\mathbb{V}_{\Lambda}^{1211}, \mathbb{V}_{\Lambda}^{2111}, \mathbb{V}_{\Lambda}^{1121}, \mathbb{V}_{\Lambda}^{1112}$ the second term involves vertices with two indices "2", like $\mathbb{V}_{\Lambda}^{1212}$ etc, which are however canceled because of the structure (30) of the Green function and single-scale propagator (31). Therefore, we find that the representations, given by the first two lines of Eq. (27) and Eqs. (30) and (31) keep their form during the flow, and the considering approach appears to be equivalent to the DMF²RG approach.

IV. THE DUAL FERMION APPROACH

The dual fermion approach of Refs. [16–19] can be conveniently formulated by splitting an effective interaction of the lattice theory (see, e.g. Ref. [23])

$$\begin{aligned} \mathcal{V}[\eta, \eta^+] &: = -\ln \int d[c, c^+] \exp \left\{ \sum_{k, \sigma} G_{0k}^{-1} (c_{k\sigma}^+ + \eta_{k\sigma}^+) (c_{k\sigma} + \eta_{k\sigma}) \right. \\ &\quad \left. - \sum_{i, \sigma} \int d\tau H_{\text{int}}[c_{i\sigma}, c_{i\sigma}^+] \right\} \\ &= -\ln Z[G_{0k}^{-1} \eta_{k\sigma}, G_{0k}^{-1} \eta_{k\sigma}^+] - \eta_{k\sigma}^+ G_{0k}^{-1} \eta_{k\sigma}, \end{aligned} \quad (32)$$

without performing its Legendre transformation. The expansion of $\mathcal{V}[\eta, \eta^+]$ in source fields generates connected (in general, one-particle reducible) Green functions, amputated by the non-interacting Green functions of the lattice theory G_{0k} . Application of covariation splitting formula to the Eq. (32) yields the relation between the lattice and dual effective interactions[33]

$$\mathcal{V}[\eta, \eta^+] = \widehat{\mathcal{V}}[\widehat{\eta}, \widehat{\eta}^+] + \sum_{k, \sigma} \eta_{k, \sigma}^+ \frac{\Sigma_{\text{loc}}(i\nu_n)}{1 - \Sigma_{\text{loc}}(i\nu_n) G_{0k}} \eta_{k, \sigma} \quad (33)$$

where the effective interaction for the dual theory is defined by

$$\begin{aligned} \widehat{\mathcal{V}}[\widehat{\eta}, \widehat{\eta}^+] &= -\ln \int D[\widetilde{c}, \widetilde{c}^+] e^{\sum_{k, \sigma} \widetilde{\mathcal{G}}_k^{-1} (\widetilde{c}_{k, \sigma}^+ - \widehat{\eta}_{k, \sigma}^+) (\widetilde{c}_{k, \sigma} - \widehat{\eta}_{k, \sigma}) - \widehat{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}^+, \widetilde{c}]}, \\ \widehat{\eta}_{k\sigma} &= \eta_{k\sigma} / [1 - \Sigma_{\text{loc}}(i\nu_n) G_{0k}], \end{aligned} \quad (34)$$

as in previous Section we have introduced $\widetilde{\mathcal{G}}_k = \mathcal{G}_k - G_{\text{loc}}$.

To introduce Λ -dependence of effective interaction, we replace again, similarly to the previous Section, $\mathcal{G}_k \rightarrow \mathcal{G}_{k, \Lambda}$, see e.g. Eqs. (16) or Eqs. (17) and (18). To generalize the relation (33) to arbitrary Λ , we also replace $G_{0k} \rightarrow G_{0k, \Lambda} := [\mathcal{G}_{k, \Lambda}^{-1} + \Sigma_{\text{loc}}(i\nu_n)]^{-1}$. The Eq. (33) then reads

$$\begin{aligned} \mathcal{V}_\Lambda[\eta, \eta^+] &= \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}_\Lambda, \widehat{\eta}_\Lambda^+] + \sum_{k, \sigma} \widehat{\eta}_{k, \Lambda, \sigma}^+ \frac{\Sigma_{\text{loc}}(i\nu_n)}{1 + \mathcal{G}_{k, \Lambda} \Sigma_{\text{loc}}(i\nu_n)} \widehat{\eta}_{k, \Lambda, \sigma}, \\ \widehat{\eta}_{k, \Lambda, \sigma} &= \eta_{k\sigma} [1 + \Sigma_{\text{loc}}(i\nu_n) \mathcal{G}_{k, \Lambda}] \end{aligned} \quad (35)$$

This allows us to perform *consistent* renormalization of the lattice and dual theory, keeping, in particular unchanged form of the relation between the dual $\Sigma_d(k, \Lambda)$ and lattice $\Sigma_{k, \Lambda}$ self-energies[16, 33]:

$$\Sigma_{k, \Lambda} = \frac{\Sigma_d(k, \Lambda)}{1 + G_{\text{loc}}(i\nu_n) \Sigma_d(k, \Lambda)} + \Sigma_{\text{loc}}(i\nu_n). \quad (36)$$

Note that the alternative way of keeping this relation is to relate the flow in the dual space directly to the flow in the real space, as it is done in Ref. [30].

The renormalization of the dual fermion effective interaction $\widehat{\mathcal{V}}_\Lambda[\widehat{\eta}, \widehat{\eta}^+]$ can be performed in the standard way. The Polchinskii equation for $\widehat{\mathcal{V}}_\Lambda$ reads:

$$\partial_\Lambda \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}, \widehat{\eta}^+] = -\Delta_{\partial_\Lambda \widetilde{G}_{k,\Lambda}} \widehat{\mathcal{V}}_\Lambda + \Delta_{\partial_\Lambda \widetilde{G}_{k,\Lambda}}^{12} \widehat{\mathcal{V}}_\Lambda^{(1)} \widehat{\mathcal{V}}_\Lambda^{(2)}$$

Note that in the latter equation the Λ -derivative does not act on the source fields $\widehat{\eta}, \widehat{\eta}^+$, which Λ -dependent values are substituted into the resulting effective interaction. The latter Λ -dependence determines the flow of the lattice effective interaction (35) according to

$$\begin{aligned} \partial_\Lambda \mathcal{V}_\Lambda[\eta, \eta^+] &= \partial_\Lambda \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}_\Lambda, \widehat{\eta}_\Lambda^+] + \left\{ \eta \frac{\delta \widehat{\mathcal{V}}_\Lambda}{\delta \widehat{\eta}_\Lambda} + \frac{\delta \widehat{\mathcal{V}}_\Lambda}{\delta \widehat{\eta}_\Lambda^+} \eta^+ \right\} (\Sigma_{\text{loc}} \partial_\Lambda G_{k,\Lambda}) \\ &\quad + \sum_{k,\sigma} \eta_{k,\sigma}^+ \Sigma_{\text{loc}}^2(i\nu_n) (\partial_\Lambda \mathcal{G}_{k,\Lambda}) \eta_{k,\sigma} \end{aligned} \quad (37)$$

Assuming

$$\begin{aligned} \mathcal{V}_\Lambda[\eta, \eta^+] &= \sum \overline{V}_{n,\Lambda} \eta_1^+ \dots \eta_{n/2}^+ \eta_{n/2+1} \dots \eta_n \\ \widehat{\mathcal{V}}_\Lambda[\widehat{\eta}, \widehat{\eta}^+] &= \sum \overline{v}_{n,\Lambda} \widehat{\eta}_1^+ \dots \widehat{\eta}_{n/2}^+ \widehat{\eta}_{n/2+1} \dots \widehat{\eta}_n \end{aligned} \quad (38)$$

this yields the standard relation between the lattice and dual two-point, Eq. (36) and higher-order vertices

$$\overline{V}_{n,\Lambda} = \overline{v}_{n,\Lambda} \prod_{i=1}^n [1 + \Sigma_{\text{loc}}(i\nu_i) \mathcal{G}_{k_i,\Lambda}] \quad (n > 2). \quad (39)$$

The latter relation accounts for the effect of the missing local self-energy insertions in the effective interaction $\widehat{\mathcal{V}}_{\text{DMFT}}[\widetilde{c}^+, \widetilde{c}]$, which determines $\widehat{\mathcal{V}}_\Lambda[\widehat{\eta}, \widehat{\eta}^+]$ according to the Eq. (34).

The Legendre transformation of $\widehat{\mathcal{V}}_\Lambda$ can be also performed in the standard way. The resulting 1PI (with respect to \widetilde{G}_k) fRG equations for the fully amputated vertex $v_\Lambda = \overline{v}_\Lambda \prod_{i=1}^4 \widetilde{\mathcal{G}}_{k_i,\Lambda} \widetilde{G}_{k_i,\Lambda}^{-1}$ ($\overline{v}_\Lambda \equiv \overline{v}_{4,\Lambda}$) read

$$\frac{d\Sigma_d}{d\Lambda} = v_\Lambda \circ S_\Lambda \quad (40)$$

$$\frac{dv_\Lambda}{d\Lambda} = v_\Lambda \circ (\widetilde{G}_\Lambda \circ S_\Lambda + S_\Lambda \circ \widetilde{G}_\Lambda) \circ v_\Lambda \quad (41)$$

where

$$\widetilde{G}_{k,\Lambda} = \widetilde{\mathcal{G}}_{k,\Lambda} / [1 - \Sigma_d(k, \Lambda) \widetilde{\mathcal{G}}_{k,\Lambda}], \quad (42)$$

$$v_\Lambda = \overline{v}_\Lambda \prod_{i=1}^4 (1 - \Sigma_d(k_i, \Lambda) \widetilde{\mathcal{G}}_{k_i,\Lambda}), \quad (43)$$

and

$$S_{k,\Lambda} = \left. \frac{d\tilde{G}_{k,\Lambda}}{d\Lambda} \right|_{\Sigma_d = \text{const}} = -(\mathcal{G}_k^{-1} - G_{\text{loc}}^{-1})\mathcal{G}_{k,\Lambda}^2 \frac{\partial f(k, \Lambda)}{\partial \Lambda} \frac{1}{[1 - \Sigma_d(k, \Lambda)\tilde{\mathcal{G}}_{k,\Lambda}]^2} \quad (44)$$

for the choice (16) and

$$S_{k,\Lambda} = \left. \frac{d\tilde{G}_{k,\Lambda}}{d\Lambda} \right|_{\Sigma_d = \text{const}} = -(\mathcal{G}_k - G_{\text{loc}}) \frac{\partial f(k, \Lambda)}{\partial \Lambda} \frac{1}{[1 - \Sigma_d(k, \Lambda)\tilde{\mathcal{G}}_{k,\Lambda}]^2}$$

for the choice (17). The initial condition reads $\Sigma_d = 0$, $V_\Lambda = \Gamma_{\text{loc}}$. As discussed above, these equation neglect the local six-point vertex, which is one-particle reducible with respect to the local Green function.

To compare the equations (40) and (41) to those of the DMF²RG approach, we consider again cutoff dependence (16). The vertices $v_{n,\Lambda}$ with $n > 2$ can be related to the corresponding vertices $V_{n,\Lambda}$ of the DMF²RG approach by amputating $\bar{V}_{n,\Lambda}$ by the respective full Green functions and using the relations (39) and (43): $V_{n,\Lambda} = \bar{V}_{n,\Lambda} \prod_{i=1}^n G_{0k_i,\Lambda} G_{k_i,\Lambda}^{-1} = v_{n,\Lambda} \prod_{i=1}^n \{[1 + \Sigma_{\text{loc}}(i\nu_i)\mathcal{G}_{k_i,\Lambda}][1 - \Sigma(k_i, \Lambda)G_{0k_i,\Lambda}]/[1 - \Sigma_d(k_i, \Lambda)\tilde{\mathcal{G}}_{k_i,\Lambda}]\}$. It can be verified that this factor cancels exactly the difference between the single-scale propagator and Green functions in the dual fermion approach [Eqs. (42) and (44)] and the DMF²RG approach [Eqs. (14) and (15)], see Ref. [30]. The corresponding equations differ however because of the Λ -derivative of the corresponding factors[30].

V. CUTOFF SCHEMES AND SELF-CONSISTENCY

Here we compare different cutoff schemes and analyze their applicability to the renormalization-group treatment, discussed in previous Sections.

We start with the simple momentum cutoff

$$f(k, \Lambda) = \theta(|\varepsilon_{\mathbf{k}}| - \Lambda) \quad (45)$$

Being combined with the Eq. (17), the choice (45) has simple physical meaning: we put the Green function equal to the local Green function inside the shell $|\varepsilon_{\mathbf{k}}| < \Lambda$ and equal to the non-local function outside this shell. This cutoff, however, does not preserve the important property of vanishing of average of \tilde{G}_Λ over momentum space during the flow:

$$\sum_{\mathbf{k}} \tilde{G}_\Lambda(\mathbf{k}, i\nu_n) = \sum_{\mathbf{k}: |\varepsilon_{\mathbf{k}}| > \Lambda} [G(k, i\nu_n) - G_{\text{loc}}(i\nu_n)] \neq 0 \quad (\Lambda > 0) \quad (46)$$

The other possible choices are the ‘interaction flow’ cutoff

$$f(k, \Lambda) = 1 - \Lambda \quad (47)$$

and frequency cutoff by C. Husemann and M. Salmhofer, Ref. [34],

$$f(k, \Lambda) = \frac{\nu_n^2}{\nu_n^2 + \Lambda^2/(1 - \Lambda)^2} \quad (48)$$

which allow to flow from the theory, non-locally non-interacting ($\Lambda = 1$) to fully interacting one ($\Lambda = 0$). These two cutoffs preserve the local part of the Green function, provided that the decomposition (17) is used. The possible disadvantage of the latter two cutoffs is the large computational effort: since one can not project momenta to the Fermi surface, one has to deal with many ‘patches’ in the whole Brillouin zone.

Finally, we comment on the effect of the self-consistency. In the dual fermion approach two ingredients of self-consistent procedure were used. The first one is obtaining the self-consistent self-energy using the diagram series in auxiliary space. This self-consistency is fully implemented in the discussed approaches via flowing self-energy. At the same time, second step (the so-called external self-consistency) requires adjusting the initial local problem according to the local part of the obtained self-energy. Similar procedure can be applied to the approaches, considered in the present paper. This type of the self-consistency is expected to be important at relatively strong coupling, where it increases the resulting self-energy, making it more “insulating”, see, e.g. Ref. [20].

VI. CONCLUSION

We have considered the application of functional renormalization-group approach to strongly-correlated electronic systems within the one-particle irreducible approach with respect to the local Green functions (1PI-LGF) and the dual fermion approach. Both mentioned approaches allow for consistent renormalization; the dual fermion approach is expected to be applicable if the one-particle reducible (with respect to the local Green functions) vertices of sixth- and higher orders are small, while the 1PI-LGF approach assumes smallness of one-particle irreducible vertices.

Further numerical investigations of the validity of these assumptions, as well as comparison of the results of the presented approaches to the flow from infinite to finite dimensions [31] to be performed.

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